

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
 Data File : BF103775.D
 Acq On : 20 Mar 2018 00:05
 Operator : JU/SJ
 Sample : J1971-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ES-6-SA-3-EW@4.5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.340	35	43	48	rVB	158446	212817	4.95%	0.543%
2	5.228	530	534	544	rVB	162541	227243	5.29%	0.579%
3	5.604	592	598	601	rBV	3788095	4212110	97.98%	10.740%
4	5.922	648	652	658	rBV	72172	68662	1.60%	0.175%
5	6.598	760	767	770	rBV	3445731	4298886	100.00%	10.961%
6	6.745	787	792	795	rBV	4002842	4210452	97.94%	10.736%
7	6.975	827	831	834	rBV	961142	861963	20.05%	2.198%
8	7.128	853	857	861	rBV	3184705	3160927	73.53%	8.060%
9	7.539	921	927	930	rBV	2440167	2712862	63.11%	6.917%
10	8.251	1044	1048	1052	rBV	1243907	1129277	26.27%	2.879%
11	9.327	1226	1231	1234	rBV	3994625	3799188	88.38%	9.687%
12	9.716	1293	1297	1300	rBV	428550	322023	7.49%	0.821%
13	9.927	1329	1333	1336	rVB	86628	66483	1.55%	0.170%
14	10.010	1343	1347	1351	rBV	1178250	1126572	26.21%	2.872%
15	10.427	1415	1418	1421	rVB	121157	88105	2.05%	0.225%
16	10.645	1450	1455	1458	rBV	35530	44173	1.03%	0.113%
17	10.804	1478	1482	1486	rBV	2301454	2319470	53.96%	5.914%
18	10.904	1496	1499	1504	rBV	89259	95630	2.22%	0.244%
19	11.504	1597	1601	1603	rBV	1123685	966126	22.47%	2.463%
20	11.527	1603	1605	1609	rVV	486154	375640	8.74%	0.958%
21	11.580	1609	1614	1617	rVB	61157	56176	1.31%	0.143%
22	11.733	1633	1640	1642	rBV2	69610	69139	1.61%	0.176%
23	12.010	1681	1687	1690	rBV2	89925	110298	2.57%	0.281%
24	12.121	1702	1706	1708	rBV2	63679	60870	1.42%	0.155%
25	12.327	1739	1741	1746	rVB2	58151	50361	1.17%	0.128%
26	12.721	1804	1808	1812	rBV	631428	526087	12.24%	1.341%
27	12.951	1841	1847	1853	rVB	460615	501030	11.65%	1.277%
28	13.092	1863	1871	1875	rBV	2994620	3076170	71.56%	7.843%
29	13.280	1900	1903	1906	rVB3	63732	54805	1.27%	0.140%
30	13.904	2004	2009	2011	rBV3	47448	58730	1.37%	0.150%
31	13.974	2016	2021	2030	rVB4	520214	551106	12.82%	1.405%
32	14.157	2047	2052	2055	rBV2	1009947	1114532	25.93%	2.842%
33	14.180	2055	2056	2064	rVB	237942	170362	3.96%	0.434%
34	14.615	2127	2130	2137	rBV3	57120	80547	1.87%	0.205%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	14.921	2178	2182	2192	rBV	784743	843239	19.62%	2.150%
36	15.233	2231	2235	2239	rBV	161122	259565	6.04%	0.662%
37	15.562	2287	2291	2297	rVB	85697	129112	3.00%	0.329%
38	15.627	2298	2302	2308	rVB	108798	144589	3.36%	0.369%
39	15.698	2308	2314	2317	rBV	543467	751919	17.49%	1.917%
40	16.215	2398	2402	2412	rVB6	66091	130447	3.03%	0.333%
41	17.256	2575	2579	2588	rVB3	45897	90071	2.10%	0.230%
42	17.345	2591	2594	2603	rVB8	41866	92112	2.14%	0.235%

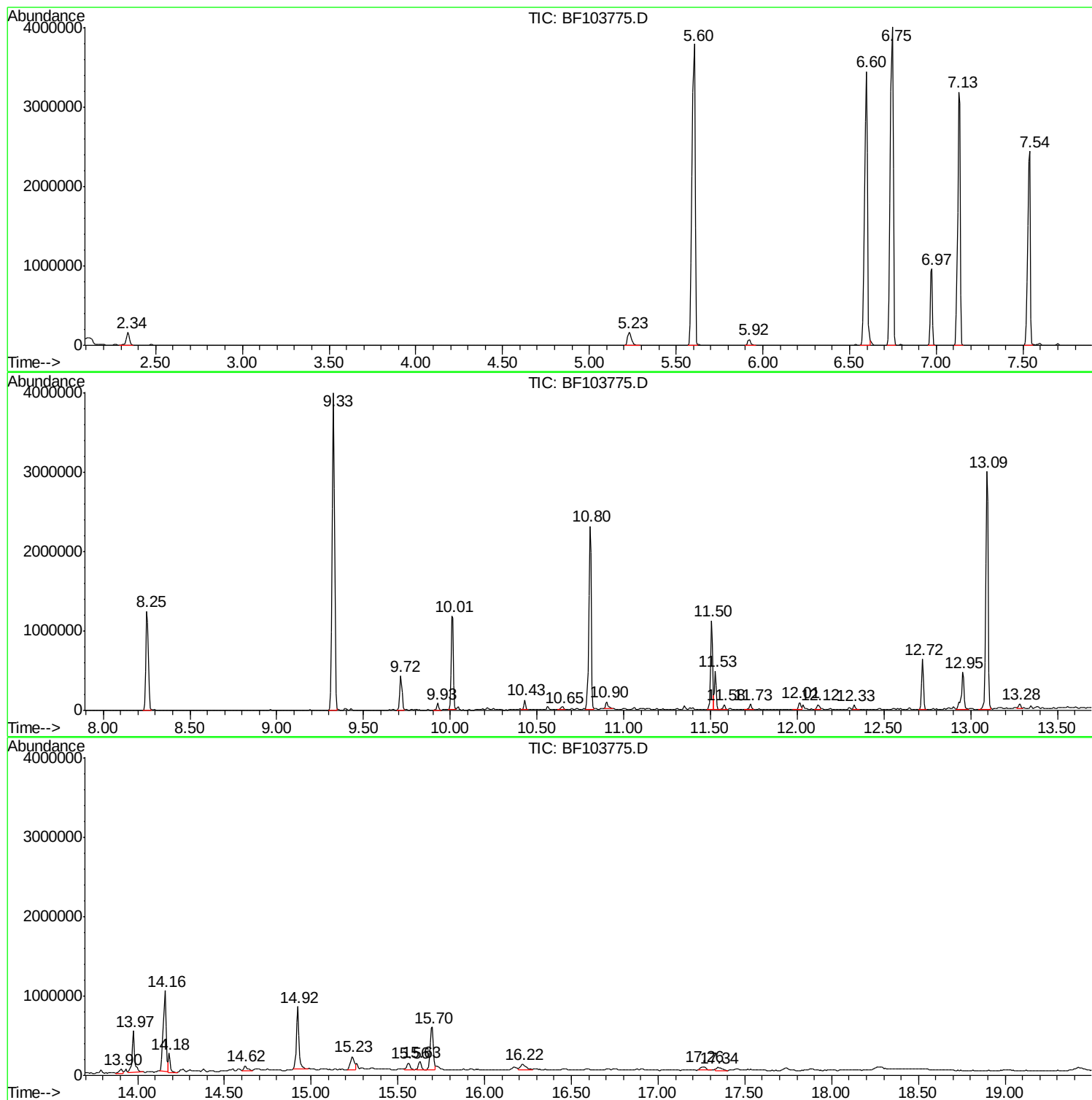
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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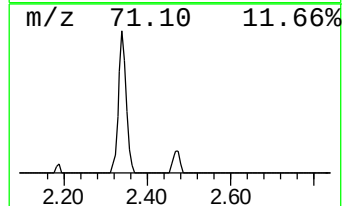
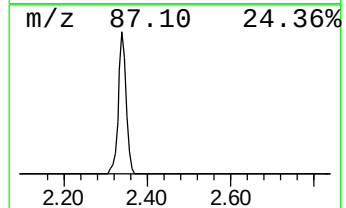
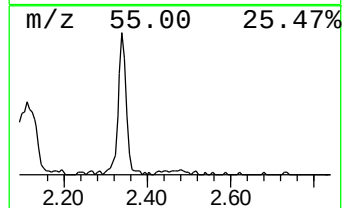
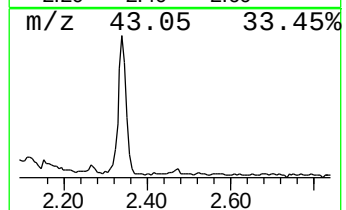
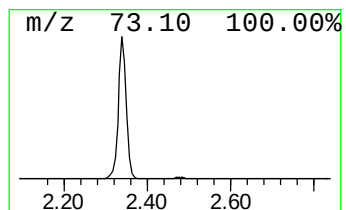
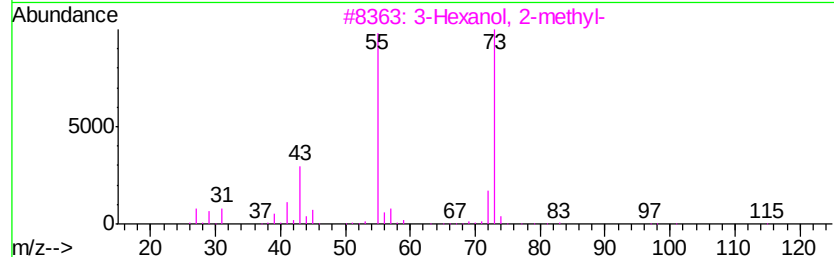
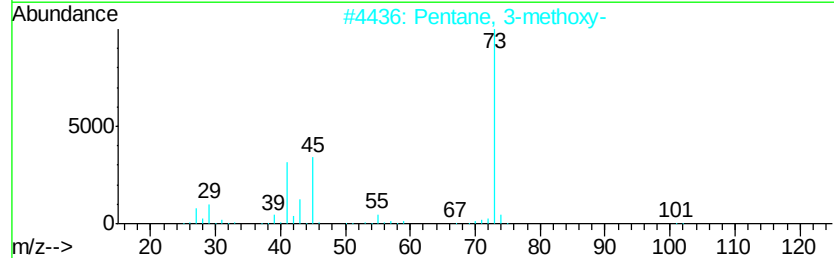
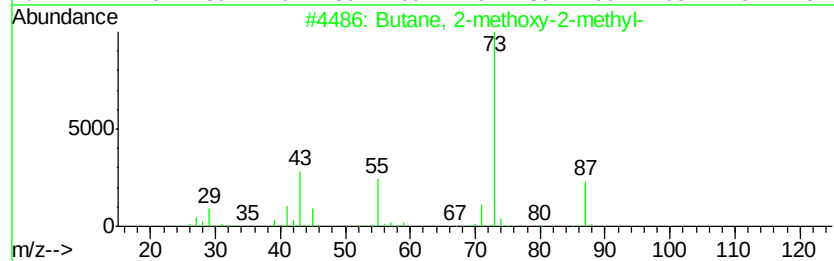
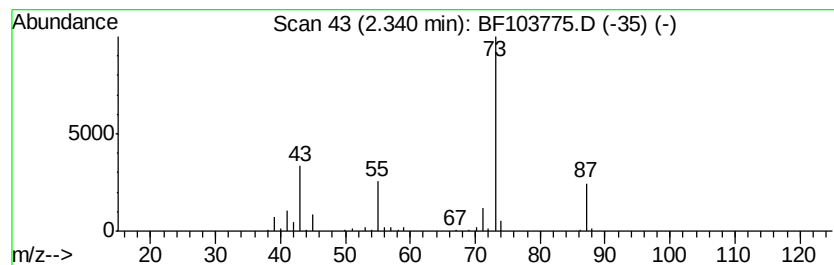
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	4.94 ng	212817	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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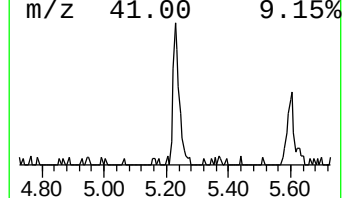
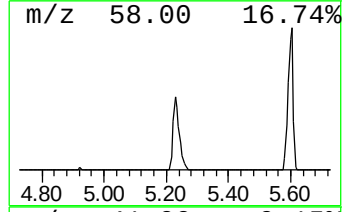
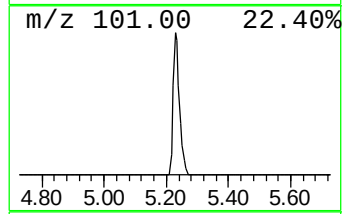
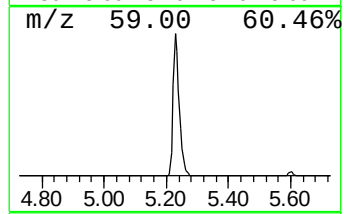
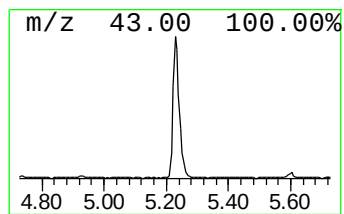
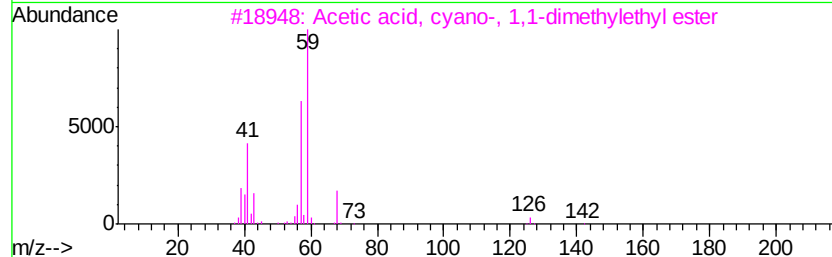
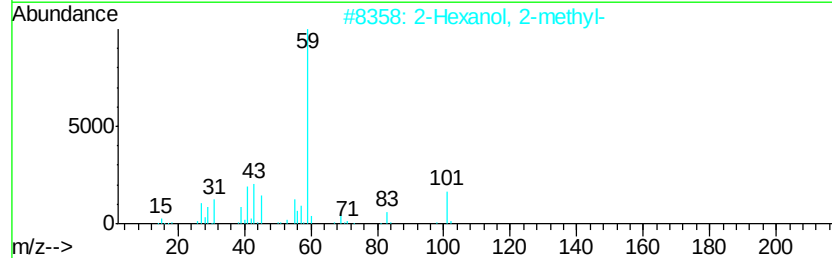
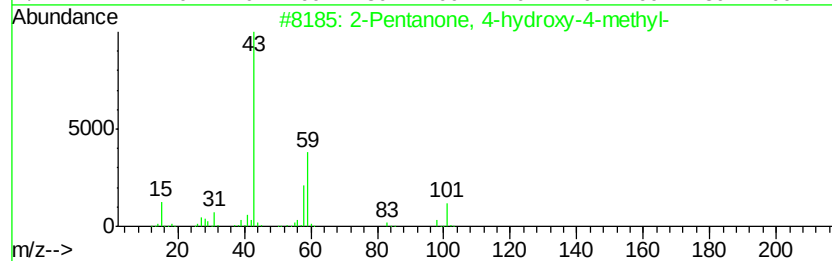
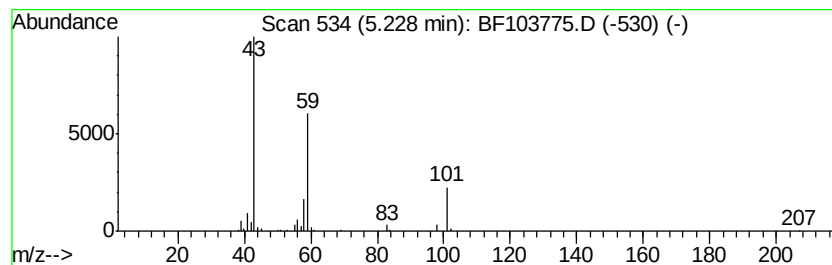
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	5.27 ng	227243	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



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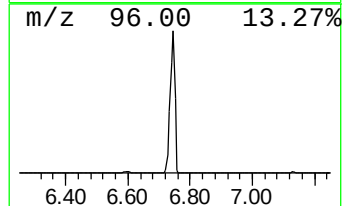
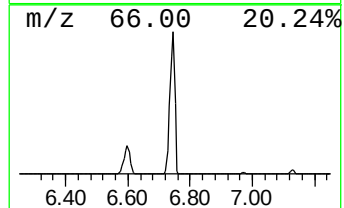
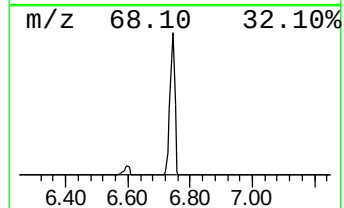
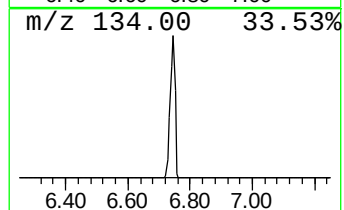
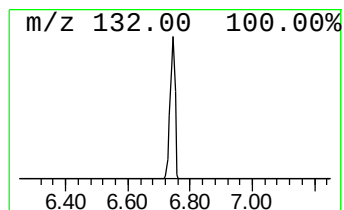
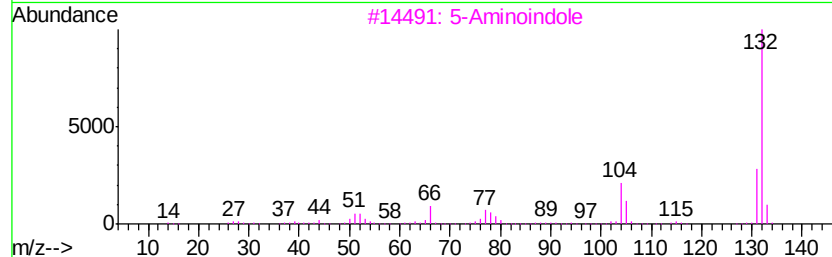
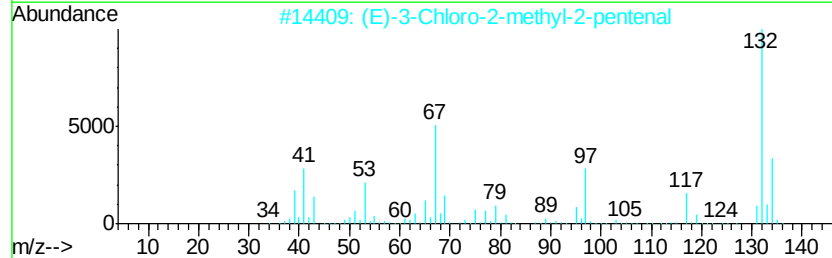
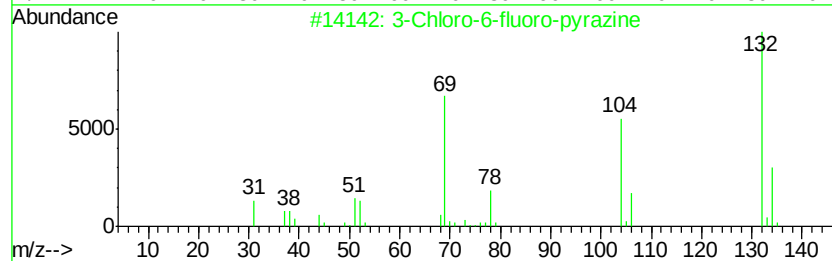
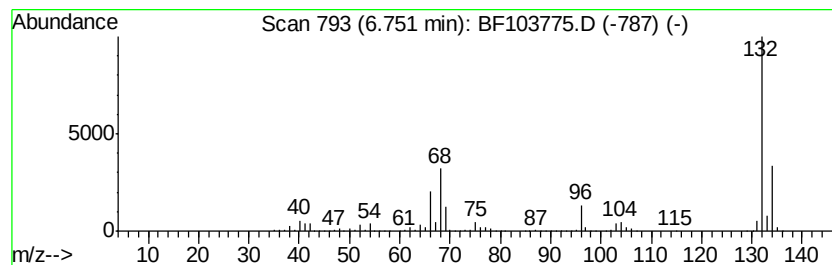
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	97.69 ng	4210450	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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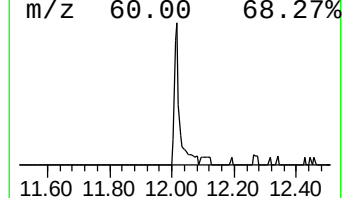
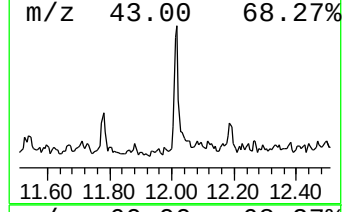
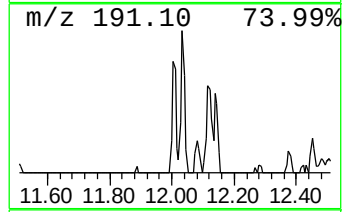
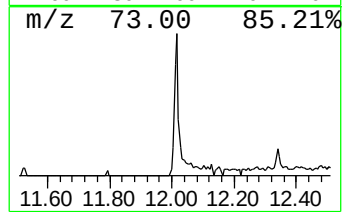
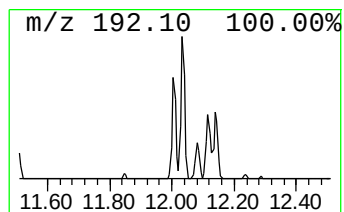
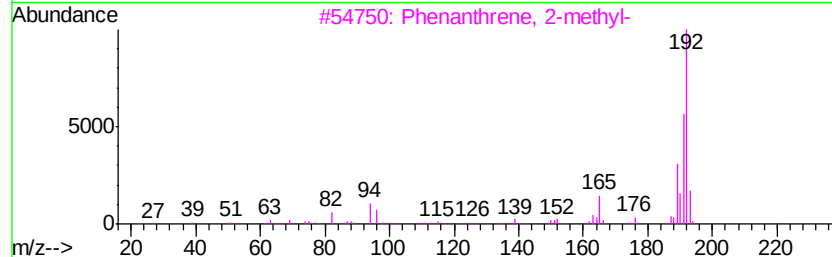
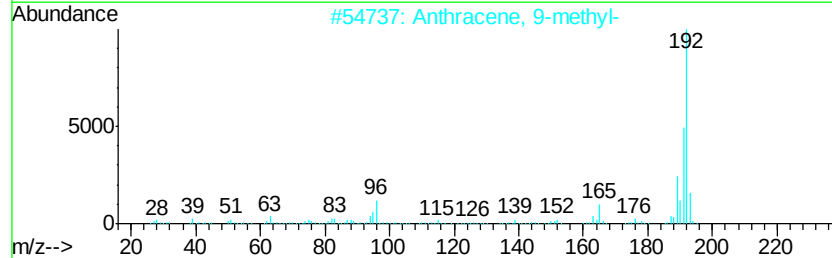
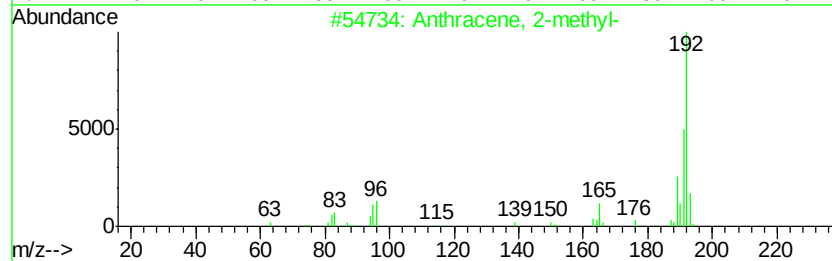
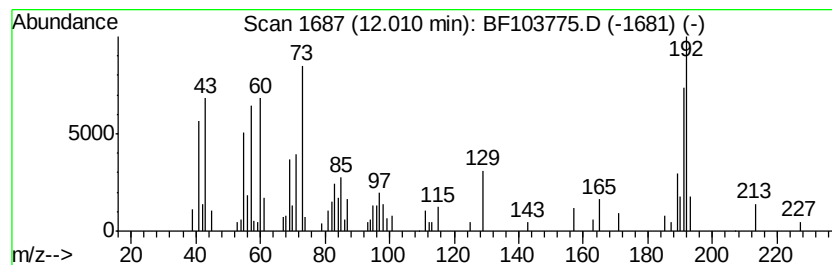
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Anthracene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.28 ng	110298	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	50
2		Anthracene, 9-methyl-	192	C15H12	000779-02-2	46
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	41
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	41
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	41



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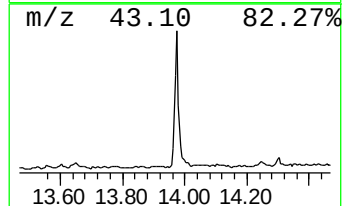
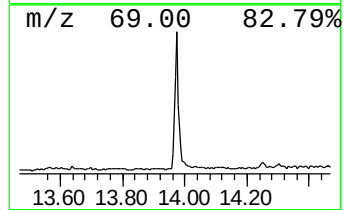
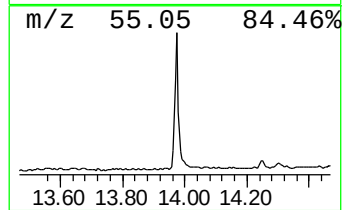
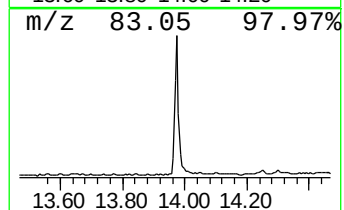
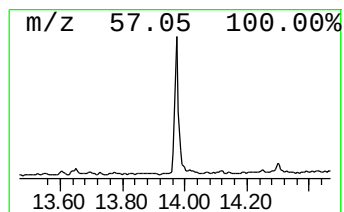
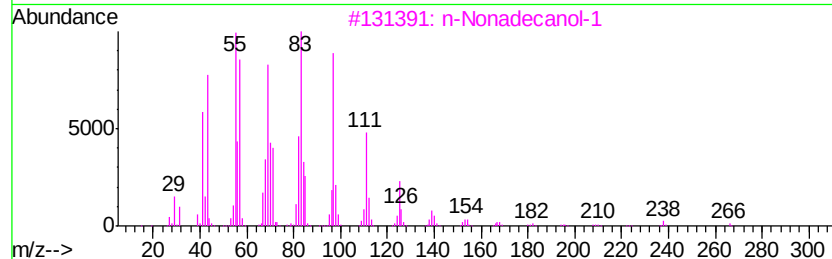
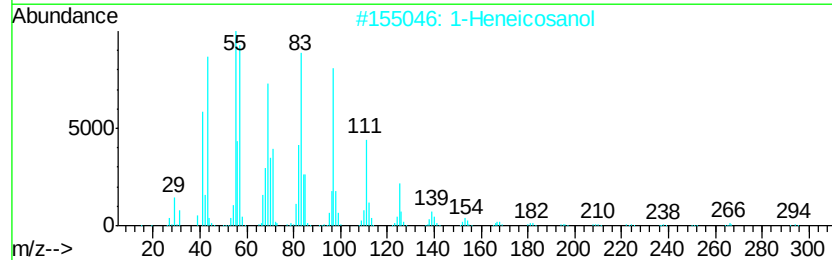
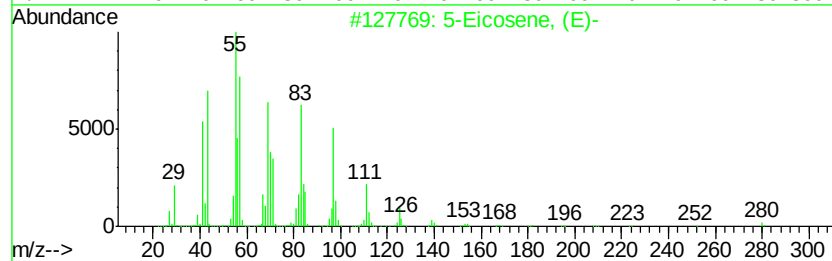
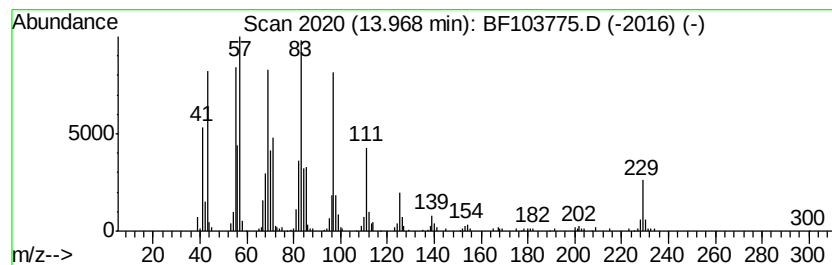
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Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	9.89 ng	551106	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103775.D
Acq On : 20 Mar 2018 00:05
Operator : JU/SJ
Sample : J1971-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ES-6-SA-3-EW@4.5

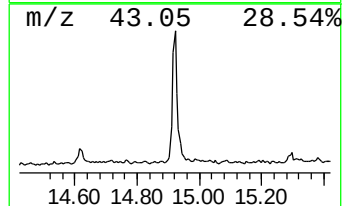
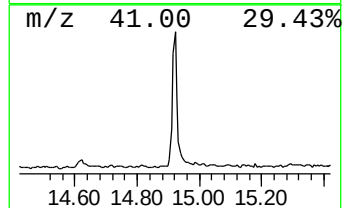
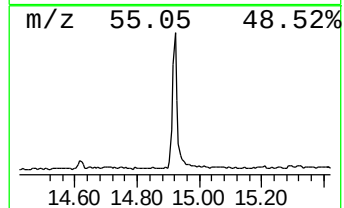
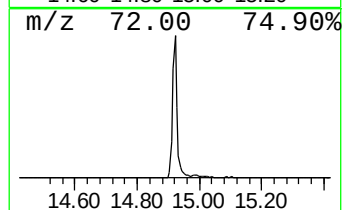
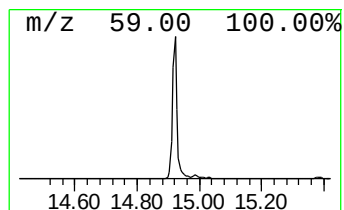
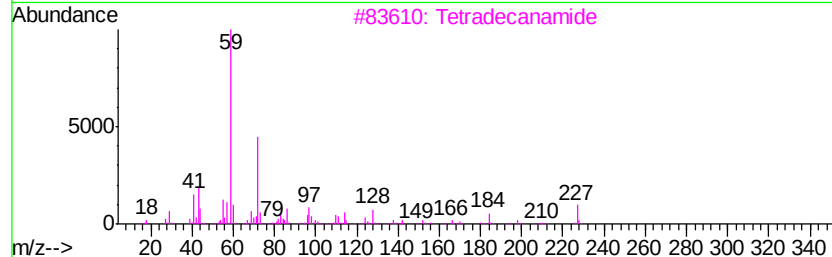
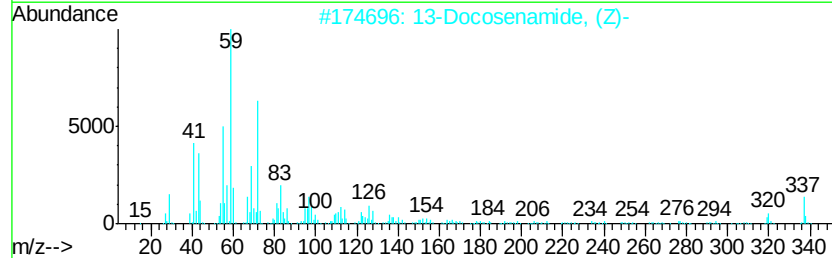
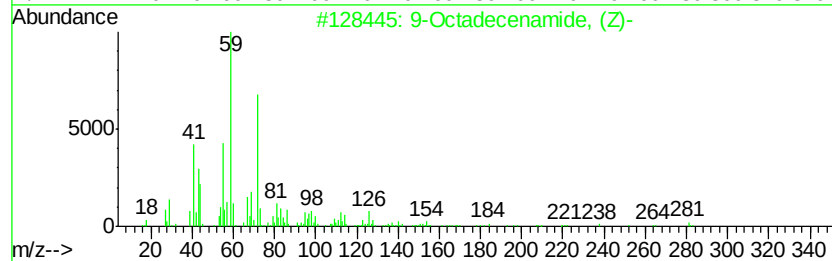
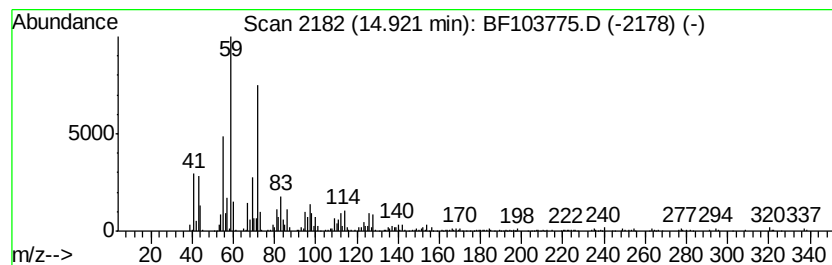
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	15.13 ng	843239	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3		Tetradecanamide	227	C14H29NO	000638-58-4	47
4		Dodecanamide	199	C12H25NO	001120-16-7	43
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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Sample : J1971-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ES-6-SA-3-EW@4.5

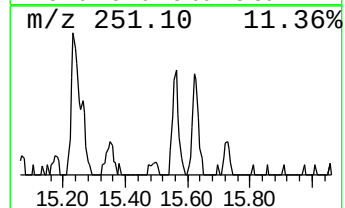
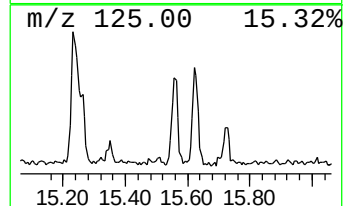
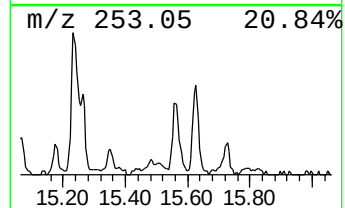
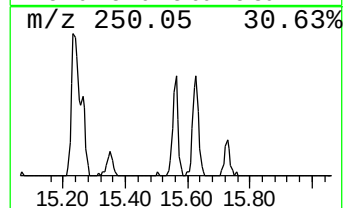
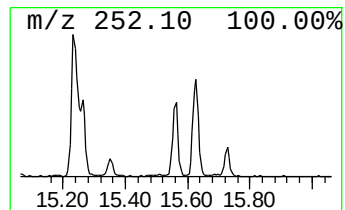
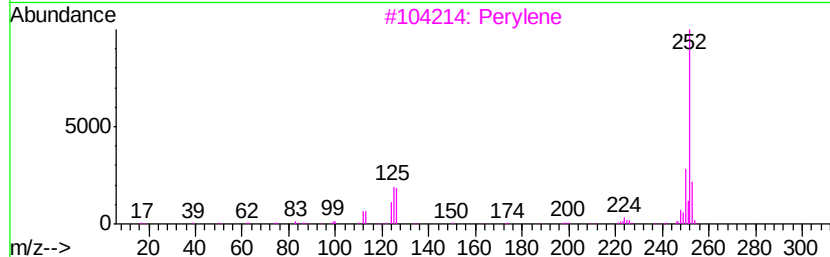
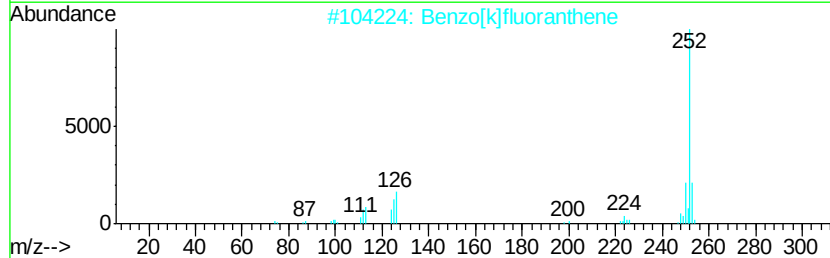
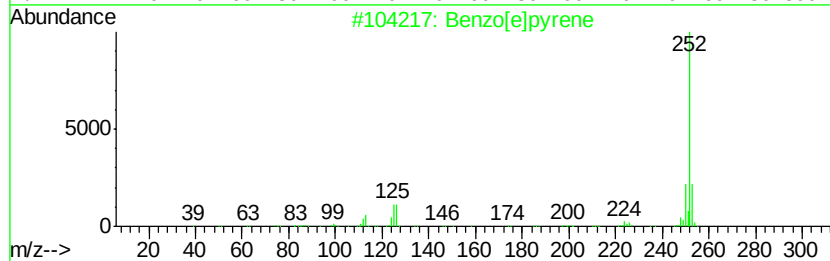
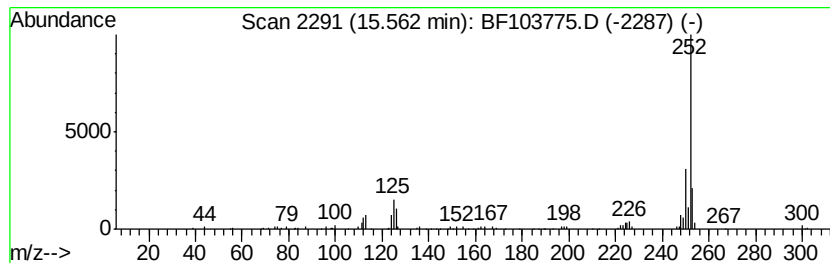
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	3.43 ng	129112	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3		Perylene	252	C20H12	000198-55-0	94
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
5		Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103775.D
Acq On : 20 Mar 2018 00:05
Operator : JU/SJ
Sample : J1971-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ES-6-SA-3-EW@4.5

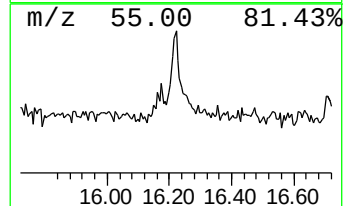
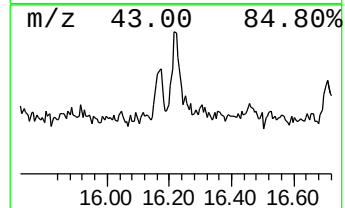
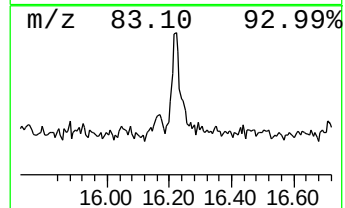
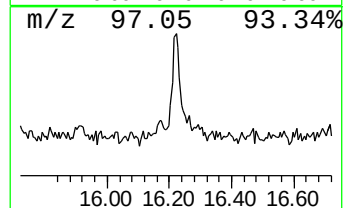
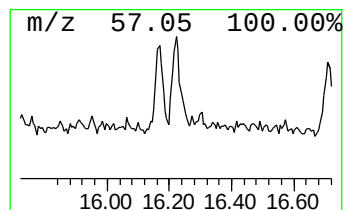
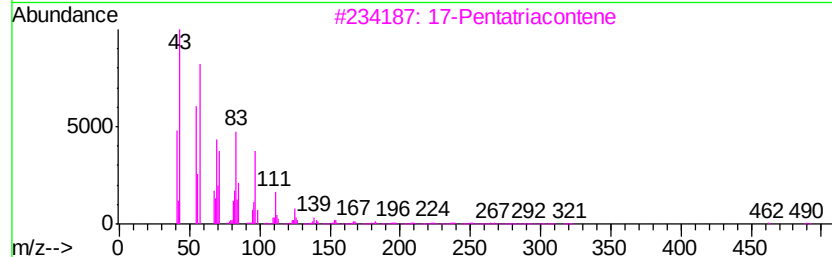
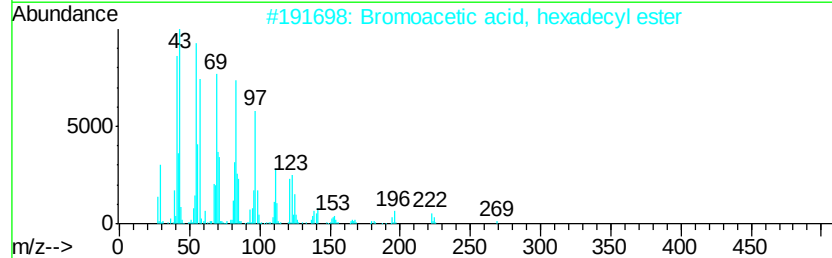
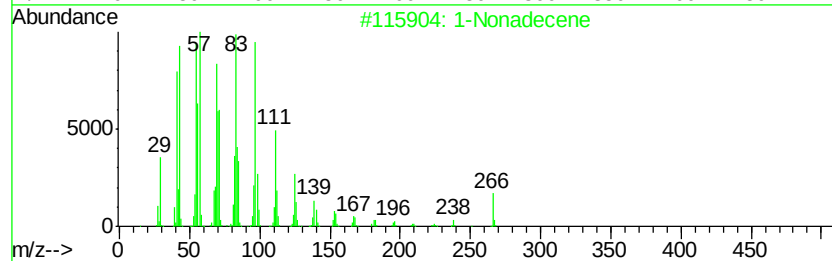
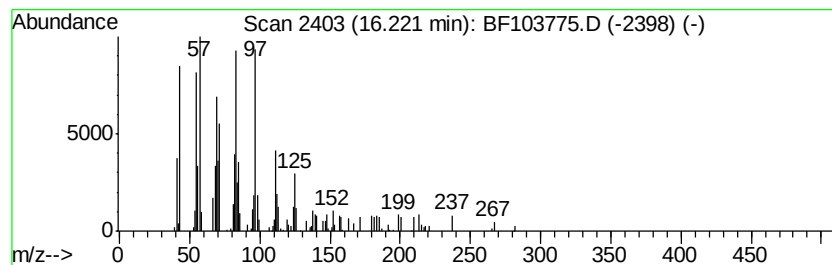
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	3.47 ng	130447	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	91
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
3		17-Pentatriacontene	491	C35H70	006971-40-0	86
4		Triacetyl acetate	480	C32H64O2	041755-58-2	83
5		Behenic alcohol	326	C22H46O	000661-19-8	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103775.D
Acq On : 20 Mar 2018 00:05
Operator : JU/SJ
Sample : J1971-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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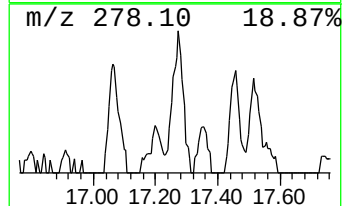
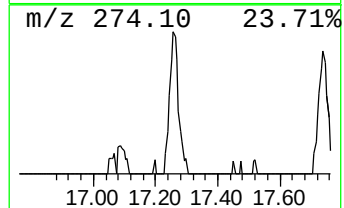
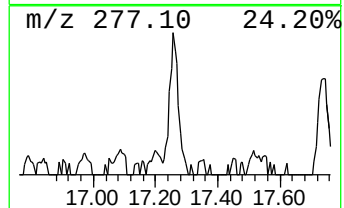
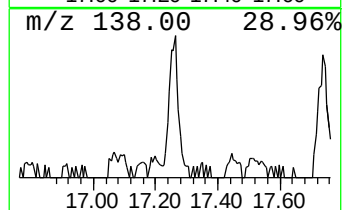
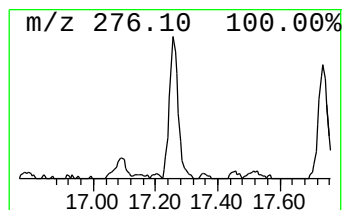
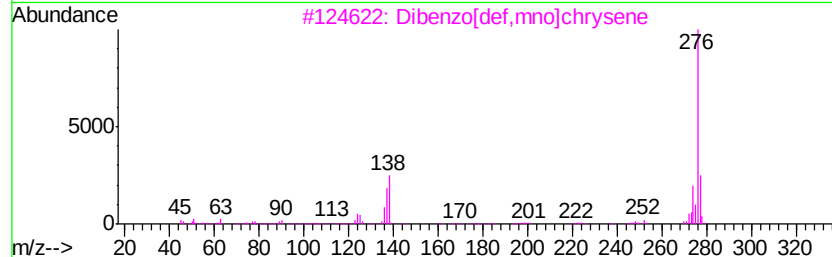
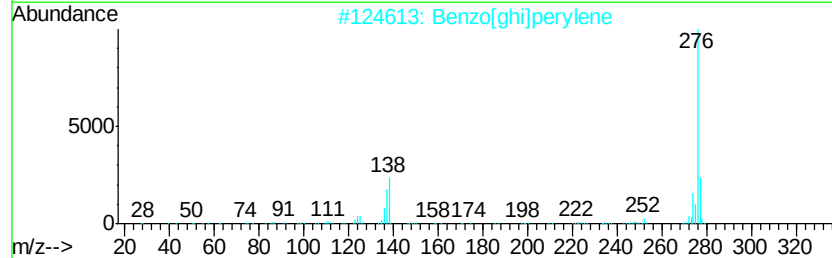
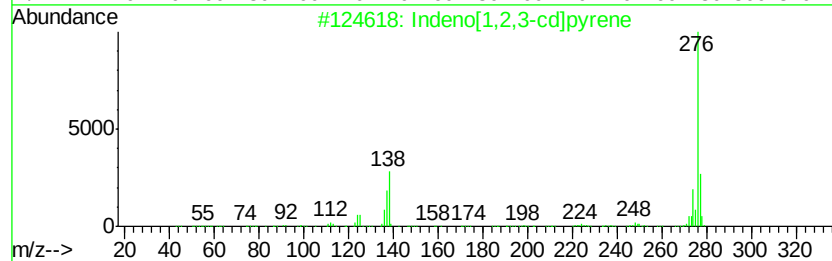
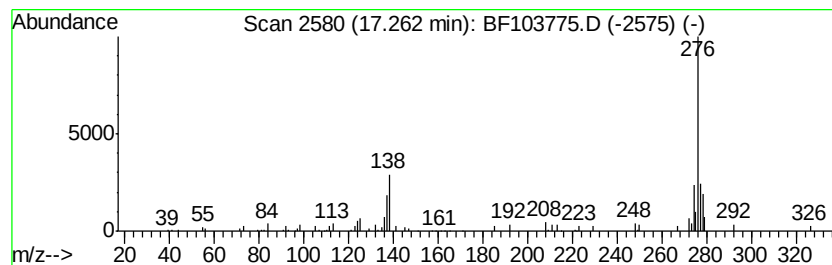
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Indeno[1,2,3-cd]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.26	2.40 ng	90071	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	95
2		Benzo[ghi]perylene	276	C22H12	000191-24-2	93
3		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
4		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	81
5		1-Naphthalenecarboxylic acid, 2-...	276	C18H12O3	038119-11-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103775.D
Acq On : 20 Mar 2018 00:05
Operator : JU/SJ
Sample : J1971-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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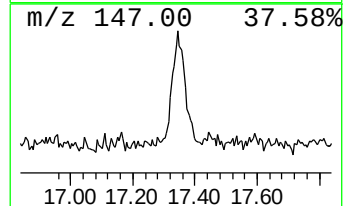
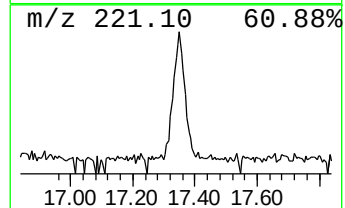
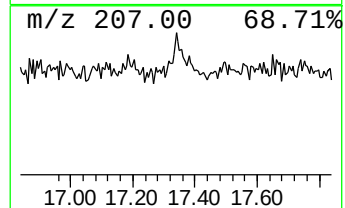
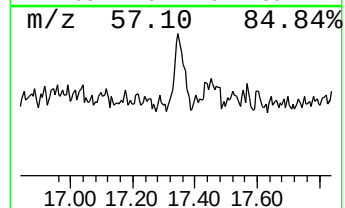
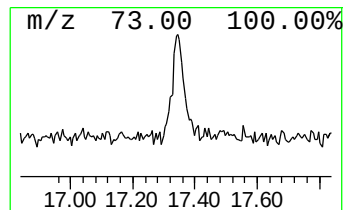
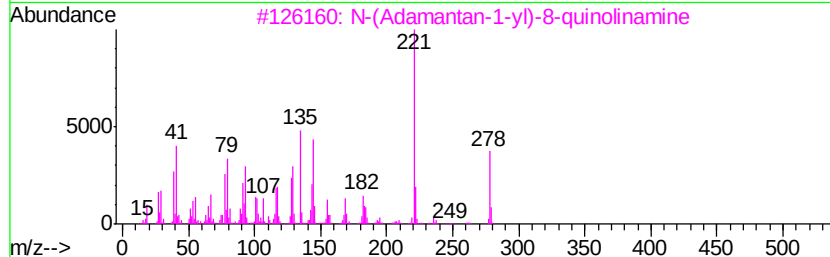
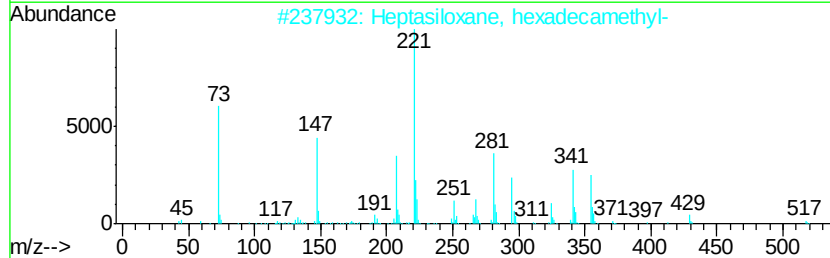
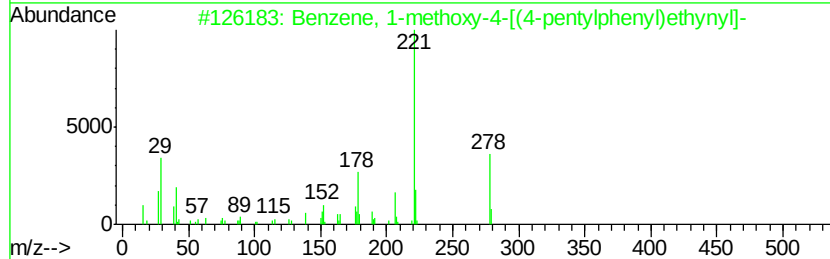
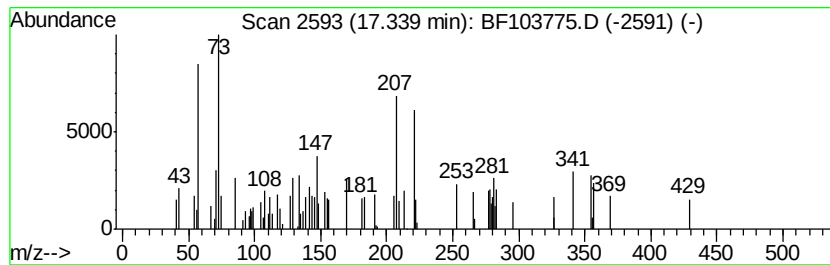
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown17.34 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.45 ng	92112	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methoxy-4-[(4-pentylp...	278	C20H22O	039969-28-3	27
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	16
3		N-(Adamantan-1-yl)-8-quinolinamine	278	C19H22N2	1000287-56-9	16
4		2-Methyl-thieno[2',3':3,4]benzo[...	221	C10H7NOS2	294668-48-7	14
5		1-[(4-Hydroxyphenyl)thioxomethyl...	221	C12H15NOS	058563-55-6	14



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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.23	5.3	ng	227243	1	6.97	861963	20.0
unknown6.75	6.75	97.7	ng	4210450	1	6.97	861963	20.0
Anthracene, 2-met...	12.01	2.3	ng	110298	4	11.50	966126	20.0
5-Eicosene, (E)-	13.97	9.9	ng	551106	5	14.16	1114530	20.0
9-Octadecenamide, ...	14.92	15.1	ng	843239	5	14.16	1114530	20.0
Benzo[e]pyrene	15.56	3.4	ng	129112	6	15.70	751919	20.0
1-Nonadecene	16.22	3.5	ng	130447	6	15.70	751919	20.0
Indeno[1,2,3-cd]p...	17.26	2.4	ng	90071	6	15.70	751919	20.0
unknown17.34	17.34	2.5	ng	92112	6	15.70	751919	20.0